

# Sufficient dimension reduction with additional information

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## Abstract

Sufficient dimension reduction is widely applied to help model building between the response  $Y$  and covariate  $X$ . While the target of interest is the relationship between  $(Y, X)$ , in some applications we also collect additional variable  $W$  that is strongly correlated with  $Y$ . From a statistical point of view, making inference about  $(Y, X)$  without using  $W$  will lose efficiency. However, it is not trivial to incorporate the information of  $W$  to infer  $(Y, X)$ . In this article, we propose a two-stage dimension reduction method for  $(Y, X)$ , that is able to utilize the additional information from  $W$ . The main idea is to confine the searching space, by constructing an envelope subspace for the target of interest. In the analysis of breast cancer data, the risk score constructed from the two-stage method can well separate patients with different survival experiences. In the Pima data, the two-stage method requires

fewer components to infer the diabetes status, while achieving higher classification accuracy than conventional method.

**Key Words:** Additional information; Central subspace; Efficiency; Envelopes; Sufficient dimension reduction.

## 1 Introduction

It is common to construct regression models or classification rules based on the observed data. Among the collected covariates, it is usually the case that some of them possess better performances than the rest in inferring the response, but with higher obtaining cost. Let  $Y \in \mathbb{R}$  be the response of interest and  $(X, W)$  be the covariates, where  $W \in \mathbb{R}$  is a better predictor of  $Y$  than  $X \in \mathbb{R}^p$ . In the breast cancer data, for instance,  $Y$  is the survival time,  $X$  contains 30 real-valued features from digitized image of a fine needle aspirate, and  $W$  is the index of breast cancer stage which is defined by tumor size and the number of lymph nodes. Obviously, the cancer stage provides more information about the survival experience, but it is an invasive process to collect  $W$ . Take the Pima data as another example,  $Y$  represents the diabetes status,  $X$  is the vector of 7 biological measurements, and  $W$  is the score of the family disease history. It is empirically shown that the family disease history is influential on the diabetes status, but may not always be available due to its frequent missingness. Consequently, although we can study the relationship between  $Y$  and  $(X, W)$ , the applicability of the constructed model is limited

since most of the collected subjects in the future are not willing to (e.g., invasive test) or not able to (e.g., missingness of the disease history) have the information of  $W$ . In this situation, the research aim is to construct a pre-screening model based on  $(Y, X)$  only. For those susceptible subjects,  $W$  is collected (with more cost) to help identify the true behavior of  $Y$  (with higher precision) for further treatment.

A common situation in modern biomedical research is the high-dimensionality of  $X$ , which makes the model building of  $(Y, X)$  difficult. Sufficient dimension reduction has been proposed to reduce the dimension of  $X$  while preserving its information for  $Y$  without requiring distributional assumption on  $(Y, X)$ . It aims to search a matrix  $\Gamma$  such that

$$Y \perp\!\!\!\perp X | \Gamma^T X. \quad (1)$$

It implies that all the information of  $X$  with respect to  $Y$  is contained in  $\Gamma^T X$ . The space  $\text{span}(\Gamma)$  is called the dimension reduction subspace for the regression of  $Y$  with respect to  $X$ . Note that (1) always holds by taking  $\Gamma$  as the identity matrix  $I_p$ , but this choice is practically useless since the dimension of  $X$  is not reduced. The central subspace (CS) induced by (1), denoted by  $\mathcal{S}_{Y|X}$ , is the intersection of all such subspaces that satisfy (1), which carries least but sufficient information of  $X$  regarding  $Y$ . In this article, we assume the existence and uniqueness of  $\mathcal{S}_{Y|X}$ , which can be guaranteed under very mild conditions (Cook, 1998). Let  $d = \dim(\mathcal{S}_{Y|X})$  be the structural dimension of  $\mathcal{S}_{Y|X}$ . The relationship of  $(Y, X)$  can be explored by the  $(d+1)$ -dimensional plot of  $(Y, \Gamma^T X)$ , which is useful to model  $(Y, X)$ . Another important concept related to this study is partial sufficient dimension reduction (Chiaromonte, Cook, and Li, 2002), which aims to find the

intersection of all subspaces  $\text{span}(\Gamma_W)$  such that

$$Y \perp\!\!\!\perp X | (\Gamma_W^T X, W). \quad (2)$$

The resulting subspace is called the partial central subspace (PCS) for the regression of  $Y$  on  $X$  given  $W$ , and is denoted by  $\mathcal{S}_{Y|X}^{(W)}$ .

Turning to the problem of constructing a model for  $(Y, X)$ , one can directly apply any dimension reduction method on  $(Y, X)$  to estimate  $\mathcal{S}_{Y|X}$ . However, this simple strategy does not utilize the information of  $W$ . As mentioned in our motivating examples,  $W$  contains more information about  $Y$  than  $X$ , and ignoring  $W$  could suffer the problem of inefficiency. This phenomenon can be partially observed through the following example.

**Example 1.1.** Let  $X \sim N(0, I_p)$  and  $W|X \sim N(\beta^T X, 1 - b^2)$  with  $b = \|\beta\| < 1$ . Let

$$\begin{aligned} Y|(X, W) &\sim N(\gamma^T X + aW, \sigma^2) \\ \Rightarrow Y|X &\sim N((\gamma + a\beta)^T X, \sigma^2 + a^2(1 - b^2)), \end{aligned} \quad (3)$$

where  $\gamma \in \mathbb{R}^p$ ,  $a \in \mathbb{R}^+$  controls the influence of  $W$  in explaining  $Y$ ,  $b$  controls the correlation between  $(X, W)$ , and  $\sigma^2$  is the conditional variance of  $Y$  given  $(X, W)$ . It gives  $\mathcal{S}_{Y|X} = \text{span}(a\beta + \gamma)$  and  $\mathcal{S}_{Y|X}^{(W)} = \text{span}(\gamma)$

One can observe from Example 1.1 that, without considering  $W$ , the conditional variance of  $Y$  is incremented by  $a^2(1 - b^2)$ , which is an increasing function of  $a$ . When  $a$  is large (i.e.,  $W$  plays an important role in affecting  $Y$ ), estimation procedure using  $(Y, X, W)$  suffers less inherent variation, and hence, has a chance of being more efficient than using  $(Y, X)$  only. Incorporating  $W$  into the estimation of  $\mathcal{S}_{Y|X}$  is not trivial. One possibility is

to use the whole data  $(Y, X, W)$  to estimate  $\mathcal{S}_{Y|X}^{(W)}$ , and see if there are certain connections between  $\mathcal{S}_{Y|X}^{(W)}$  and  $\mathcal{S}_{Y|X}$ . Chiaromonte, Cook, and Li (2002) show that either  $W \perp\!\!\!\perp X | \Gamma_W^T X$  or  $W \perp\!\!\!\perp Y | \Gamma_W^T X$  implies  $\mathcal{S}_{Y|X} \subseteq \mathcal{S}_{Y|X}^{(W)}$ , and  $W \perp\!\!\!\perp Y | X$  implies  $\mathcal{S}_{Y|X}^{(W)} \subseteq \mathcal{S}_{Y|X}$ . However, the stated conditions are not easy to check in practice, and  $\mathcal{S}_{Y|X} \neq \mathcal{S}_{Y|X}^{(W)}$  in general. In Example 1.1, for instance,  $\mathcal{S}_{Y|X}^{(W)} = \text{span}(\gamma)$  is different from the target of interest  $\mathcal{S}_{Y|X} = \text{span}(a\beta + \gamma)$ . The aim of this study is to propose a dimension reduction method that targets  $\mathcal{S}_{Y|X}$  correctly, while utilizing all the information of  $(Y, X, W)$ .

The rest of this article is organized as follows. In Section 2 we review some dimension reduction methods. A two-stage estimation procedure for  $\mathcal{S}_{Y|X}$  that utilizes  $W$  is introduced in Section 3. Sections 4-5 conduct numerical studies to show the superiority of the proposed method. The paper is ended with a discussion in Section 6.

## 2 Reviews of Dimension Reduction Methods

### 2.1 Preliminary

In the rest of discussion,  $Y$  is assumed to be a discrete random variable with finite support  $(1, \dots, H)$ . For the continuous case, the discretization procedure of Li (1991) can be applied. For the purpose of illustration,  $W$  is also assumed to be a discrete random variable with finite support  $(1, \dots, C)$ . Extensions to general  $W$  will be discussed. Let  $Z = \Sigma^{-1/2}(X - \mu)$  with  $\mu = E[X]$  and  $\Sigma = \text{cov}(X)$  be the standardized version of  $X$ . There is no difference in considering the dimension reduction problem for  $X$  and  $Z$ , due to the relationships  $\mathcal{S}_{Y|X} = \Sigma^{-1/2}\mathcal{S}_{Y|Z}$  and  $\mathcal{S}_{Y|X}^{(W)} = \Sigma^{-1/2}\mathcal{S}_{Y|Z}^{(W)}$ . For convenience, we will work

on the  $Z$ -scale to introduce our method and transform back to the  $X$ -scale. In practice,  $Z$  is replaced by  $\widehat{Z} = \widehat{\Sigma}^{-1/2}(X - \widehat{\mu})$ , where  $\widehat{\mu}$  and  $\widehat{\Sigma}$  are moment estimators of  $\mu$  and  $\Sigma$ . Let  $\{(Y_i, X_i, W_i)\}_{i=1}^n$  be random copies of  $(Y, X, W)$ . Let  $P_A$  be the orthogonal projection matrix onto a space  $A$ , or  $\text{span}(A)$  when  $A$  stands for a matrix, and  $Q_A = I - P_A$ .  $I(\cdot)$  is the indicator function. For a population quantity  $\theta$ ,  $\widehat{\theta}$  or  $\widetilde{\theta}$  denotes its sample version. In the subsequent discussion, we assume that all the structural dimensions (e.g.,  $d$ ) are known first, and their selections will be discussed separately.

## 2.2 Estimation of $\mathcal{S}_{Y|Z}$

One branch of dimension reduction methods is to search a kernel matrix  $K_{Y|Z}$  satisfying  $\text{span}(K_{Y|Z}) = \mathcal{S}_{Y|Z}$ . The solutions from the maximization problem

$$\max_{\substack{\beta_s: \|\beta_s\|=1 \\ \beta_s^T \beta_l = 0 \forall s \neq l}} \sum_{k=1}^d \beta_k^T \widehat{K}_{Y|Z} \beta_k \quad (4)$$

are used to estimate a basis of  $\mathcal{S}_{Y|Z}$ . Inverse regression-based methods usually rely on the linearity condition  $E[Z|A^T Z] = P_A Z$  for first-order methods, such as sliced inverse regression (SIR) of Li (1991), and further require the constant variance condition  $\text{cov}(Z|A^T Z) = Q_A$  for second-order methods, such as sliced average variance estimates (SAVE) of Cook and Weisberg (1991).

Undoubtedly, SIR is the most widely applied dimension reduction method. The population kernel matrix of SIR is  $K_{\text{SIR}} = \text{cov}(E[Z|Y])$ . Its sample version is

$$\widehat{K}_{\text{SIR}} = \sum_{h=1}^H \frac{n_h}{n} m_h m_h^T, \quad (5)$$

where  $m_h = \frac{1}{n_h} \sum_{i=1}^n \widehat{Z}_i I(Y_i = h)$  is the slice mean and  $n_h = \sum_{i=1}^n I(Y_i = h)$  is the size of the slice  $h$ . Under the linearity condition, Li (1991) shows that the span of the leading  $d$  eigenvectors of  $\widehat{K}_{\text{SIR}}$  is a  $\sqrt{n}$ -consistent estimator of  $\mathcal{S}_{Y|Z}$ . SIR has the drawback of not being able to identify  $\mathcal{S}_{Y|Z}$  when  $E[Z|Y]$  is degenerate, and SAVE is proposed to solve this problem (but requires both the linearity and the constant variance conditions). The kernel matrix of SAVE is given by  $K_{\text{SAVE}} = E\{I - \text{cov}(Z|Y)\}^2$ . At the sample level, the leading eigenvectors of

$$\widehat{K}_{\text{SAVE}} = \sum_{h=1}^H \frac{n_h}{n} \{I - \widehat{\text{cov}}(Z|Y = h)\}^2 \quad (6)$$

is used to estimate  $\mathcal{S}_{Y|Z}$ , where  $\widehat{\text{cov}}(Z|Y = h)$  is the sample covariance matrix of  $\widehat{Z}_i$  within the slice  $h$ .

### 2.3 Estimation of $\mathcal{S}_{Y|Z}^{(W)}$

When the target of interest is  $\mathcal{S}_{Y|Z}^{(W)}$ , Chiaromonte, Cook, and Li (2002) propose the partial sliced inverse regression (PSIR). Let  $(Y_w, Z_w)$  denote the random variables  $(Y, Z)$  given  $W = w$ , and let  $Z_w^* = \Sigma_w^{-1/2}(Z_w - \mu_w)$  with  $\mu_w = E[Z_w]$  and  $\Sigma_w = \text{cov}(Z_w)$  being the standardized version of  $Z_w$  under  $\{W = w\}$ . The rationale of PSIR can be seen from the decomposition

$$\mathcal{S}_{Y|Z}^{(W)} = \bigoplus_{w=1}^C \mathcal{S}_{Y_w|Z_w} = \bigoplus_{w=1}^C \Sigma_w^{-1/2} \mathcal{S}_{Y_w|Z_w^*} = \Sigma_0^{-1/2} \bigoplus_{w=1}^C \mathcal{S}_{Y_w|Z_w^*}, \quad (7)$$

where the first equality is from Proposition 3.3 of Chiaromonte, Cook, and Li (2002) and the last equality holds under the equal covariance condition  $\Sigma_w = \Sigma_0, w = 1, \dots, C$ . Let

$\hat{\mu}_w$  and  $\hat{\Sigma}_w$  be the moment estimators of  $\mu_w$  and  $\Sigma_w$ ,  $\Sigma_0$  is estimated by  $\hat{\Sigma}_0 = \sum_{w=1}^C \frac{n_w}{n} \hat{\Sigma}_w$ ,

where  $n_w$  is the number of samples within  $\{W = w\}$ . Let

$$\hat{K}_{\text{PSIR}} = \sum_{w=1}^C \frac{n_w}{n} \hat{K}_w^*, \quad (8)$$

where  $\hat{K}_w^*$  is the kernel matrix of SIR based on  $(Y_w, \hat{Z}_w^*)$ , and  $\hat{Z}_w^* = \hat{\Sigma}_0^{-1/2}(\hat{Z}_w - \hat{\mu}_w)$ . A basis of  $\mathcal{S}_{Y|Z}^{(W)}$  can be estimated by  $\hat{\Sigma}_0^{-1/2}$  multiplying the leading eigenvectors of  $\hat{K}_{\text{PSIR}}$ .

### 3 Estimation of $\mathcal{S}_{Y|Z}$ with Additional Information

#### 3.1 The $W$ -envelope subspace and a two-stage method

As mentioned in Section 1 that  $W$  contains useful information regarding  $Y$ , and our aim is to incorporate  $W$  into the estimation procedure of  $\mathcal{S}_{Y|Z}$ . The basic idea is to use  $(Y, Z, W)$  to construct an *envelope* that encapsulates the searching space of  $\mathcal{S}_{Y|Z}$ . With the confined searching space, we have a chance to improve efficiency. The construction of such an envelope is based on the fact that

$$\mathcal{S}_{Y|Z} \subseteq \mathcal{S}_{(Y,W)|Z}, \quad (9)$$

where the equality holds since  $Y$  is a function of  $(Y, W)$ . The inclusion property provides a way to utilize the information of  $W$ , via constructing the *W-envelope subspace*.

**Definition 3.1.** *The  $W$ -envelope subspace of  $\mathcal{S}_{Y|Z}$  is defined to be  $\mathcal{S}_{\text{env}} = \mathcal{S}_{(Y,W)|Z}$  with the structural dimension  $d_{\text{env}} = \dim(\mathcal{S}_{\text{env}})$ .*

Again, we assume that  $d_{\text{env}}$  is known and its selection will be discussed later. Another expression of  $\mathcal{S}_{\text{env}}$  via the concept of PCS is established below.



**Proposition 3.1.**  $\mathcal{S}_{\text{env}} = \mathcal{S}_{Y|Z}^{(W)} \oplus \mathcal{S}_{W|Z}$ .

Although two expressions of  $\mathcal{S}_{\text{env}}$  are equivalent in the population level, we will see that the expression  $\mathcal{S}_{\text{env}} = \mathcal{S}_{Y|Z}^{(W)} \oplus \mathcal{S}_{W|Z}$  provides a more robust manner to construct  $\mathcal{S}_{\text{env}}$ . Since  $\mathcal{S}_{(Y,W)|Z}$  must exist, we always have the inclusion relationship

$$\mathcal{S}_{Y|Z} \subseteq \mathcal{S}_{\text{env}}. \quad (10)$$

Take Example 1.1 to exemplify, where  $\mathcal{S}_{Y|Z} = \text{span}(a\beta + \gamma)$ ,  $\mathcal{S}_{W|Z} = \text{span}(\beta)$ , and  $\mathcal{S}_{Y|Z}^{(W)} = \text{span}(\gamma)$  due to  $\text{cov}(X) = I_p$ . It can be seen that  $\mathcal{S}_{Y|Z}$  is a proper subspace of  $\mathcal{S}_{\text{env}} = \text{span}([\beta, \gamma])$ .

Reasonably, it suffices to search  $\mathcal{S}_{Y|Z}$  within  $\mathcal{S}_{\text{env}}$  due to (10). An improved estimation procedure is to search a basis of  $\mathcal{S}_{Y|Z}$  via solving the maximization problem

$$\max_{\substack{\beta_s: \beta_s \in \mathcal{S}_{\text{env}} \\ \|\beta_s\|=1, \beta_s^T \beta_l = 0 \ \forall \ s \neq l}} \sum_{k=1}^d \beta_k^T \hat{K}_{Y|Z} \beta_k. \quad (11)$$

Different from (4), the estimation criterion (11) incorporates the information of  $W$  via adding the constraints  $\beta_s \in \mathcal{S}_{\text{env}}$ . Let  $B_{\text{env}}$  be a basis of  $\mathcal{S}_{\text{env}}$ . From Proposition 3 of Naik and Tsai (2005), the solutions of (11) are derived to be the leading  $d$  eigenvectors of

$$P_{B_{\text{env}}} \hat{K}_{Y|Z} P_{B_{\text{env}}}. \quad (12)$$

Observe from (12) that, instead of searching a basis of  $\mathcal{S}_{Y|Z}$  in  $\mathbb{R}^p$ , we first project  $\hat{K}_{Y|Z}$  onto  $\mathcal{S}_{\text{env}}$  within which we search a basis of  $\mathcal{S}_{Y|Z}$ . See Figure 1 for a conceptual display. Since  $\mathcal{S}_{\text{env}}$  is rarely known a priori, we need to estimate  $P_{B_{\text{env}}}$  before estimating  $\mathcal{S}_{Y|Z}$  from (12). Let  $K_{\text{env}}$  be a positive semi-definite kernel matrix satisfying  $\text{span}(K_{\text{env}}) = \mathcal{S}_{\text{env}}$ ,

and let  $\widehat{B}_{\text{env}}$  be the leading  $\nu$  ( $\nu \geq d_{\text{env}}$ ) eigenvectors of  $\widehat{K}_{\text{env}}$ . The two-stage estimation procedure for  $\mathcal{S}_{Y|Z}$  is proposed to be the leading  $d$  eigenvectors of

$$P_{\widehat{B}_{\text{env}}} \widehat{K}_{Y|Z} P_{\widehat{B}_{\text{env}}}. \quad (13)$$

Obviously, the construction of  $\widehat{K}_{\text{env}}$  based on  $(Y, Z, W)$  plays the key role to the performance of the two-stage method, wherein the information of  $W$  should be properly utilized. This issue will be discussed in Section 3.2.

### 3.2 The construction of $\widehat{K}_{\text{env}}$

We now proceed to the construction of  $\widehat{K}_{\text{env}}$ , the critical part of the two-stage method. One approach is to use the expression  $\mathcal{S}_{\text{env}} = \mathcal{S}_{(Y,W)|Z}$  directly. Let  $K_{(Y,W)|Z}$  be a positive semi-definite kernel matrix satisfying  $\text{span}(K_{(Y,W)|Z}) = \mathcal{S}_{(Y,W)|Z}$ . Then, one can use  $\widehat{K}_{\text{env}} = \widehat{K}_{(Y,W)|Z}$  in the construction of the two-stage method, and any existing dimension reduction method can be applied to obtain  $\widehat{K}_{(Y,W)|Z}$ . For example,  $K_{(Y,W)|Z}$  can be chosen to be the SIR kernel matrix  $K_{\text{SIR}}^* = \text{cov}(E[Z|Y, W])$ . In the sample level, one can still use (5) to construct  $\widehat{K}_{\text{SIR}}^*$ , except  $(Y, W)$  are now treated as the response to do slicing. A naive two-stage estimator for  $\mathcal{S}_{Y|Z}$  is proposed below.

**Definition 3.2.** *The two-stage estimator of  $\mathcal{S}_{Y|Z}$  using the leading  $\nu$  eigenvectors of  $\widehat{K}_{\text{env}} = \widehat{K}_{(Y,W)|Z}$  is defined to be  $\widehat{B}_0(\nu)$ .*

The efficiency gain of  $\widehat{B}_0(\nu)$  is guaranteed when the dimension is correctly specified at  $\nu = d_{\text{env}}$ , which supports the superiority of the two-stage method. Let  $\widetilde{B}$  be the direct estimator of  $\mathcal{S}_{Y|Z}$  based on  $(Y, Z)$ . We have the following result.

**Proposition 3.2.** *Assume the linearity and constant variance conditions. Consider  $\widehat{K}_{Y|Z} = \widehat{K}_{\text{SIR}}$ . Then,  $\widehat{B}_0(d_{\text{env}})$  with  $\widehat{K}_{(Y,W)|Z} = \widehat{K}_{\text{SIR}}^*$  is asymptotically more efficient than  $\widetilde{B}$  in estimating  $\mathcal{S}_{Y|Z}$ , provided that  $\text{span}(K_{\text{SIR}}) \cap \text{span}(K_{\text{SIR}}^* - K_{\text{SIR}}) \neq \{0\}$ .*

*Proof.* By treating  $(Y, W)$  as the response and considering the function  $g(Y, W) = Y$ , the result is a direct consequence of Theorem 1 of Hung (2012).  $\square$

The naive two-stage estimator  $\widehat{B}_0(\nu)$  can be improved. One advantage of using  $\widehat{K}_{\text{env}} = \widehat{K}_{(Y,W)|Z}$  is its simple implementation, which can be conducted by existing algorithms with slight modification. However, this method does not consider the relative importance of  $\mathcal{S}_{Y|Z}^{(W)}$  and  $\mathcal{S}_{W|Z}$  when forming  $\mathcal{S}_{\text{env}}$ . For instance, in the case of  $W \perp\!\!\!\perp Z$ ,  $\mathcal{S}_{W|Z} = \{0\}$  and is useless to improve estimating  $\mathcal{S}_{Y|Z}$ . Using  $\widehat{K}_{\text{env}} = \widehat{K}_{(Y,W)|Z}$  cannot adapt to this situation and, hence, may loss efficiency in estimating  $\mathcal{S}_{\text{env}}$  and  $\mathcal{S}_{Y|Z}$ . The problem can be solved by constructing  $\widehat{K}_{\text{env}}$  via the alternative expression  $\mathcal{S}_{\text{env}} = \mathcal{S}_{Y|Z}^{(W)} \oplus \mathcal{S}_{W|Z}$ . Let  $K_{Y|Z}^{(W)}$  and  $K_{W|Z}$  be two positive semi-definite kernel matrices satisfying  $\text{span}(K_{Y|Z}^{(W)}) = \mathcal{S}_{Y|Z}^{(W)}$  and  $\text{span}(K_{W|Z}) = \mathcal{S}_{W|Z}$ . From Proposition 3.1, we have for any  $\xi \in (0, 1)$  that

$$\mathcal{S}_{\text{env}} = \text{span} \left( \xi \cdot K_{W|Z} + (1 - \xi) \cdot K_{Y|Z}^{(W)} \right). \quad (14)$$

A more robust method is to construct  $\widehat{K}_{\text{env}}$  by the hybrid kernel matrix

$$\widehat{K}(\xi) = \xi \cdot \widehat{K}_{W|Z} + (1 - \xi) \cdot \widehat{K}_{Y|Z}^{(W)}, \quad (15)$$

where  $\xi$  controls the relative importance of  $\widehat{K}_{W|Z}$  and  $\widehat{K}_{Y|Z}^{(W)}$  in estimating  $\mathcal{S}_{\text{env}}$ . Observe that the construction of  $\widehat{K}_{W|Z}$  is still a dimension reduction problem for  $Z$ , where  $W$  is now treated as a response. Hence, we can apply SIR to construct  $\widehat{K}_{W|Z}$  as in (5) with  $Y$

being replaced by  $W$ . As to  $\widehat{K}_{Y|Z}^{(W)}$ , it is nothing but a partial dimension reduction problem, and PSIR can be applied. An improved two-stage estimator for  $\mathcal{S}_{Y|Z}$  is proposed below.

**Definition 3.3.** *The two-stage estimator of  $\mathcal{S}_{Y|Z}$  using the leading  $\nu$  eigenvectors of  $\widehat{K}_{\text{env}} = \widehat{K}(\xi)$  is defined to be  $\widehat{B}(\nu, \xi)$ .*

We note that any dimension reduction method can be applied to construct  $\widehat{K}_{\text{env}}$ , and is not limited to SIR and PSIR.

**Remark 3.4.** *For multivariate  $W$ , one can still apply PSIR to construct  $\widehat{K}_{Y|Z}^{(W)}$  by using  $W$  to do slicing. As to the construction of  $\widehat{K}_{(Y,W)|Z}$  or  $\widehat{K}_{W|Z}$ , this is a dimension reduction problem with multivariate response, and the projective resampling technique (Li, Wen, and Zhu, 2008) can be applied. With these modifications, the same two-stage procedure is ready to estimate  $\mathcal{S}_{Y|Z}$  by using the modified  $\widehat{K}_{\text{env}}$ .*

### 3.3 Determination of $(d, d_{\text{env}})$

To estimate the structural dimension, Li (1991) proposes an asymptotic test based on the sum of the tail eigenvalues of the kernel matrix. This method, however, requires the asymptotic distribution of eigenvalues, which is complicated when  $Z$  is not normally distributed. Cook and Yin (2001) suggest a permutation test to determine the structural dimension, but it requires heavy computational load. Alternatively, we adopt a BIC-type criterion to select  $(d, d_{\text{env}})$ , which is modified from the criterion of Zhu *et al.* (2010). Let

$$\widehat{d}_{\text{env}}(\xi) = \underset{k=1, \dots, p}{\operatorname{argmax}} \left\{ \frac{\sum_{j=1}^k \{\ln(\widehat{\lambda}_j + 1) - \widehat{\lambda}_j\}}{\sum_{j=1}^p \{\ln(\widehat{\lambda}_j + 1) - \widehat{\lambda}_j\}} - \frac{C_n}{n} \left( pk - \frac{k(k-1)}{2} \right) \right\}, \quad (16)$$

where  $\hat{\lambda}_j$  is the  $j$ -th eigenvalue of  $\hat{K}_{\text{env}}$ ,  $C_n$  is a pre-determined penalty, and  $pk - \frac{k(k-1)}{2}$  is the number of parameters required to specify a  $p \times p$  symmetric matrix with rank  $k$ . Note that  $\hat{d}_{\text{env}}(\xi)$  can be a function of  $\xi$ , depending on the choices of  $\hat{K}_{\text{env}} = \hat{K}(\xi)$  or  $\hat{K}_{\text{env}} = \hat{K}_{(Y,W)|Z}$ . To integrate out the effect of  $\xi$ , we propose to estimate  $d_{\text{env}}$  by

$$\hat{d}_{\text{env}} = \text{median} \left\{ \hat{d}_{\text{env}}(\xi) : \xi \in \Xi \right\}. \quad (17)$$

The same idea can be applied to determine  $d$ . Let

$$\hat{d}(\xi) = \underset{k=1, \dots, \hat{d}_{\text{env}}(\xi)}{\text{argmax}} \left\{ \frac{\sum_{j=1}^k \{\ln(\hat{\lambda}_j^* + 1) - \hat{\lambda}_j^*\}}{\sum_{j=1}^p \{\ln(\hat{\lambda}_j^* + 1) - \hat{\lambda}_j^*\}} - \frac{C_n}{n} \left( pk - \frac{k(k-1)}{2} \right) \right\}, \quad (18)$$

where  $\hat{\lambda}_j^*$  is the  $j$ -th eigenvalue of  $P_{\hat{B}_{\text{env}}} \hat{K}_{Y|Z} P_{\hat{B}_{\text{env}}}$  with  $\nu = \hat{d}_{\text{env}}(\xi)$ . We then propose to estimate  $d$  by

$$\hat{d} = \text{median} \left\{ \hat{d}(\xi) : \xi \in \Xi \right\}. \quad (19)$$

For any fixed  $\xi$ , the consistency of  $\hat{d}_{\text{env}}(\xi)$  and  $\hat{d}(\xi)$  can be similarly derived as Theorem 4 of Zhu *et al.* (2010), provided  $C_n/n \rightarrow 0$  and  $C_n \rightarrow \infty$  as  $n \rightarrow \infty$ . Since  $\Xi$  is finite, the consistency of  $(\hat{d}, \hat{d}_{\text{env}})$  is a direct consequence.

## 4 Numerical Studies

### 4.1 Simulation settings

We consider two models for simulations. The first one is model (3) in Example 1.1 with  $\beta = b \cdot (0, 0, 1, 1, 0_{p-4})^T / \sqrt{2}$  and  $\gamma = (1, 1, 0, 0, 0_{p-4})^T / \sqrt{2}$ , which gives  $\mathcal{S}_{Y|Z} = \text{span}(a\beta + \gamma)$  and  $\mathcal{S}_{\text{env}} = \text{span}([\beta, \gamma])$ . The second model is constructed as below. Let  $X \sim$

$N(0, I_p)$  and  $W = (W_1, W_2)$  be generated from  $W_1|X \sim N(\beta_1^T X, 1 - \|\beta_1\|^2)$  and  $W_2|X \sim N(\beta_2^T X, 1 - \|\beta_2\|^2)$ , where  $\beta_1 = b \cdot (0, 0, 1, 1, 0_{p-4})^T / \sqrt{2}$  and  $\beta_2 = b \cdot (1, 1, 0, 0, 0_{p-4})^T / \sqrt{2}$ .

Condition on  $(X, W)$ ,  $Y$  is generated from

$$\begin{aligned} Y|(X, W) &\sim N((1 + \alpha^T X)(aW_1 + aW_2 + \gamma^T X), \sigma^2) \\ \Rightarrow Y|X &\sim N((1 + \alpha^T X)(a\beta_1 + a\beta_2 + \gamma)^T X, \sigma^2 + 2a^2(1 - b^2)(1 + \alpha^T X)^2) \end{aligned} \quad (20)$$

with  $\alpha = (0, 0, 0, 0, 1, 1, 0_{p-6}^T)^T / \sqrt{2}$  and  $\gamma = (1, 1, 2, 2, 0_{p-4}^T)^T / \sqrt{10}$ . The setting is designed so that  $\gamma \in \text{span}([\beta_1, \beta_2])$ , i.e.,  $\mathcal{S}_{Y|Z}^{(W)} = \text{span}([\alpha, \gamma])$  and  $\mathcal{S}_{W|Z} = \text{span}([\beta_1, \beta_2])$  have overlap. It gives  $\mathcal{S}_{Y|Z} = \text{span}([\alpha, a(\beta_1 + \beta_2) + \gamma])$  and  $\mathcal{S}_{\text{env}} = \text{span}([\alpha, \beta_1, \beta_2])$ . Note that in both models,  $a$  controls the ability of  $W$  to explain  $Y$ , and  $b$  controls the correlation between  $W$  and  $Z$ .

Simulation data is generated from two settings of  $(n, p) = (150, 9)$  and  $(250, 25)$ . Both  $\hat{B}$  and  $\hat{B}_0$  are conducted to compare with the direct method  $\tilde{B}$ . We use SIR to construct  $\hat{K}_{Y|Z}$  by categorizing  $Y$  into 10 slices. For  $\hat{B}$ , we use SIR to construct  $\hat{K}_{W|Z}$  by categorizing each component of  $W$  into 2 and 3 slices for the cases of  $n = 150$  and  $n = 250$ , respectively, and use PSIR to construct  $\hat{K}_{Y|Z}^{(W)}$  by further categorizing  $Y$  into 3 slices within each slice of  $W$ . For  $\hat{B}_0$ , SIR is used to construct  $\hat{K}_{(Y,W)|Z}$  using the same slicing as  $\hat{B}$ . We also try other settings of slices, which give similar results and thus are not reported. For the two-stage method, we use  $C_n = n^{1/4}$  and  $\Xi = \{\frac{5}{50}, \frac{6}{30}, \dots, \frac{45}{50}\}$  to determine  $(\nu^*, \xi^*)$ . The *trace correlation coefficient* (Hooper, 1959)  $r = \sqrt{\text{tr}(P_{B_1}P_{B_2})/d}$  of two  $d$ -dimensional subspaces with bases  $B_1$  and  $B_2$  is used as the performance measure. The value of  $r$  belongs to  $[0, 1]$ , and  $r = 1$  indicates  $\text{span}(B_1) = \text{span}(B_2)$ . Simulation

results are reported under  $\sigma = 0.5$  and different combinations of  $a = (0, 0.5, \dots, 3)$  and  $b = (0.1, 0.3)$ , based on  $m = 300$  bootstraps and 500 replicates.

## 4.2 Simulation results

We first compare the performances of the two-stage method  $\hat{B}$  and the direct method  $\tilde{B}$  when  $d$  is known. Simulation results under models (3) and (20) are placed in Figures 2-3 (a)-(b), which show the means of the trace correlation  $\hat{r}$  and  $\tilde{r}$  of  $\hat{B}$  and  $\tilde{B}$ , respectively. Recall that  $a$  controls the influence of  $W$  on  $Y$ , and  $b$  controls the correlation between  $(Z, W)$ . Thus, in the absence of  $W$ ,  $\tilde{r}$  decreases as  $a$  increases. For any fixed  $a$ , we can also observe a high  $\tilde{r}$  for large  $b$ , since in this situation  $Z$  can well predict  $Y$  through  $W$ . A similar pattern can be observed for  $\hat{r}$ , since  $\hat{B}$  is obtained from modifying  $\hat{K}_{Y|Z}$ .

The magnitude of improvement  $(\hat{r} - \tilde{r})$  shows a different behavior. One can see that  $(\hat{r} - \tilde{r})$  increases as  $a$  increases. The more information  $W$  contains (i.e., large  $a$ ), the more improvement  $\hat{B}$  can achieve. On the other hand,  $(\hat{r} - \tilde{r})$  increases as  $b$  decreases. Note that when  $b$  is small,  $Z$  can hardly be a surrogate of  $W$  and, hence, the two-stage method benefits more from utilizing  $W$ . Overall,  $\hat{B}$  outperforms  $\tilde{B}$  in all settings.

The trace correlation  $\hat{r}_0$  of  $\hat{B}_0$  is also shown in Figures 2-3 (a)-(b). One can obviously see that the winner is still  $\hat{B}$ , followed by  $\hat{B}_0$  and then  $\tilde{B}$ . These results further indicate the benefit of using a hybrid method to estimate  $\mathcal{S}_{\text{env}}$  via  $K_{Y|Z}^{(W)}$  and  $K_{W|Z}$ . Indeed, we rarely know the relative importance of  $K_{Y|Z}^{(W)}$  and  $K_{W|Z}$ , which is totally ignored when directly estimating  $\mathcal{S}_{\text{env}}$  by  $\hat{K}_{(Y,W)|Z}$ . By using the hybrid kernel matrix  $\hat{K}(\xi)$ , it allows the data to select  $\xi$  with minimal variability to adapt to various relationships between

$K_{Y|Z}^{(W)}$  and  $K_{W|Z}$ , and a good performance of  $\hat{B}$  is achieved.

The simulation results of  $\hat{d}$  using  $\hat{K}_{\text{env}} = \hat{K}(\xi)$  and different  $C_n$  values are placed in Table 1, which shows the selection proportions under four settings of two models with  $(n, p) = (150, 9)$ . The results of  $\tilde{d}$ , the estimator of  $d$  from using  $\hat{K}_{Y|Z}$  directly, are also shown for comparisons. One can see that  $\hat{d}$  achieves higher accuracies than  $\tilde{d}$  over a wide range of  $C_n$ . By incorporating  $W$ , we cannot only improve estimating  $\mathcal{S}_{Y|Z}$ , but also improve the selection consistency for the structural dimension  $d$ .

## 5 Data Analysis

### 5.1 The Pima Indians diabetes data

The data contains females of Pima Indian heritage, each with 7 biological covariates, 1 covariate of family disease history, and an indicator of diabetes status. Detailed description of the data can be found in Smith *et al.* (1988). After removing observations with missing values, there are 392 patients remained. In our analysis, we take the score of the family disease history as  $W$ , which is shown to have strong association with diabetes status ( $Y$ ). However, missingness is very likely to occur when collecting  $W$ , which limits its usage in future applications. It is thus of interest to construct prediction rule for the diabetes status based solely on the rest biological measurements ( $X$ ).

Since SIR can only find one direction for binary response, we use SAVE to construct  $\hat{K}_{Y|Z}$ . As to the estimation of  $\mathcal{S}_{\text{env}}$ , we apply PSIR to construct  $\hat{K}_{Y|Z}^{(W)}$ , and apply SIR to construct  $\hat{K}_{W|Z}$ . In this analysis, we choose  $(\nu, \xi)$  of the two-stage method via maximiz-



ing the leave-one-out classification accuracy (CA) from quadratic discriminant analysis (Rencher, 1995), which gives  $\widehat{B} = \widehat{B}(4, 0.2)$ . The maximum leave-one-out CA is 0.7959 for  $(\widehat{S}_1, \widehat{S}_2)$ , while it is 0.7041 for  $(\widetilde{S}_1, \widetilde{S}_2)$ , and is 0.7781 for  $(\widetilde{S}_1, \widetilde{S}_2, \widetilde{S}_3)$ . It indicates an efficiency gain from using  $W$ . This fact can be further observed from the scatter plots of  $\widehat{S}_i$  and  $\widetilde{S}_i$  in Figure 4. One can see that  $(\widetilde{S}_1, \widetilde{S}_2)$  tend to separate diabetes status by variation, while different locations of two groups are detected for  $\widetilde{S}_3$ . Interestingly,  $(\widehat{S}_1, \widehat{S}_2, \widehat{S}_3)$  demonstrate different behaviors in that patients with different diabetes status tend to have different variations of  $\widehat{S}_1$ , while different locations are observed for  $\widehat{S}_2$ . Moreover,  $\widehat{S}_3$  is useless in separating the diabetes status, suggesting that one only requires  $(\widehat{S}_1, \widehat{S}_2)$  to infer the diabetes status. However, it requires  $(\widetilde{S}_1, \widetilde{S}_2, \widetilde{S}_3)$  when ignoring  $W$ . By utilizing  $W$ , the order of the “location-separating component” is also changed from  $\widetilde{S}_3$  to  $\widehat{S}_2$ .

Following the procedure of Li (2006), we also implement the quadratic discriminant analysis to classify subjects by using  $W$  together with the leading two components of  $\widehat{K}_{Y|Z}^{(W)}$ . The result is treated as the benchmark since  $W$  is directly used in the classification process. The resulting leave-one-out CA for the benchmark method is 0.7985. By using the two-stage procedure, we only require two dimension reduction components of biological measurements to infer the behavior of diabetes status, and can achieve comparable performance as the benchmark method.

## 6 Discussion

In this article, we propose a general framework to utilize the additional information of  $W$  to improve estimating  $\mathcal{S}_{Y|Z}$ , via constructing the  $W$ -envelope subspace  $\mathcal{S}_{\text{env}}$ .

The central mean subspace  $\mathcal{S}_{E[Y|X]}$  is the minimum subspace  $\text{span}(\Gamma_m)$  such that  $E[Y|X] = E[Y|\Gamma_m^T X]$ . Obviously, we must have  $\mathcal{S}_{E[Y|X]} \subseteq \mathcal{S}_{Y|X}$ . Therefore,  $\mathcal{S}_{Y|X}$  may contain redundant directions to infer  $E[Y|X]$ , and  $\mathcal{S}_{E[Y|X]}$  should be the target when the research interest is the conditional mean  $E[Y|X]$ . The idea of  $\mathcal{S}_{E[Y|X]}$  is first proposed by Cook and Li (2002), wherein the estimation method is also developed. Later, Xia *et al.* (2002) propose the minimum average variance estimation (MAVE), which is based on local linear smoothers and does not require strong assumptions on the distribution of  $X$ . With the presence of  $W$ , an interesting question is how to utilize  $W$  to improve the estimation of  $\mathcal{S}_{E[Y|X]}$ . By definition, we have the inclusion property

$$\mathcal{S}_{E[Y|Z]} \subseteq \mathcal{S}_{Y|Z} \subseteq \mathcal{S}_{\text{env}}.$$

It implies that the idea of the envelope subspace  $\mathcal{S}_{\text{env}}$  can still be applied, to confine the searching space of  $\mathcal{S}_{E[Y|X]}$  and, hence, to enhance the estimation efficiency. Although the idea is straightforward, efforts should be made to adapt to different estimation criteria (such as MAVE) for  $\mathcal{S}_{E[Y|X]}$ .

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Table 1: Selection proportions of  $\hat{d}$  and  $\tilde{d}$  under models (3) and (20) with different combinations of  $(a, b, C_n)$ . The columns correspond to the true dimension  $d$  are marked as bold.

model	$(a, b)$		$C_n = 0.5n^{1/4}$				$C_n = n^{1/4}$				$C_n = 2n^{1/4}$			
			1	2	3	> 3	1	2	3	> 3	1	2	3	> 3
(3)	(1, 0.1)	$\hat{d}$	<b>.365</b>	.625	.010	.000	<b>.855</b>	.145	.000	.000	<b>.985</b>	.015	.000	.000
		$\tilde{d}$	<b>.000</b>	.010	.500	.490	<b>.000</b>	.205	.735	.060	<b>.005</b>	.790	.205	.000
	(1, 0.3)	$\hat{d}$	<b>.470</b>	.520	.010	.000	<b>.885</b>	.115	.000	.000	<b>.995</b>	.005	.000	.000
		$\tilde{d}$	<b>.000</b>	.005	.540	.455	<b>.000</b>	.205	.750	.045	<b>.005</b>	.870	.125	.000
	(3, 0.1)	$\hat{d}$	<b>.015</b>	.490	.485	.010	<b>.075</b>	.855	.070	.000	<b>.480</b>	.520	.000	.000
		$\tilde{d}$	<b>.000</b>	.000	.030	.970	<b>.000</b>	.000	.265	.735	<b>.000</b>	.080	.715	.205
	(3, 0.3)	$\hat{d}$	<b>.010</b>	.650	.335	.005	<b>.165</b>	.795	.040	.000	<b>.660</b>	.340	.000	.000
		$\tilde{d}$	<b>.000</b>	.000	.055	.945	<b>.000</b>	.005	.475	.520	<b>.000</b>	.135	.810	.055
	(1, 0.1)	$\hat{d}$	.000	<b>.480</b>	.520	.000	.010	<b>.905</b>	.085	.000	.110	<b>.890</b>	.000	.000
		$\tilde{d}$	.000	<b>.005</b>	.175	.820	.000	<b>.010</b>	.625	.365	.000	<b>.210</b>	.765	.025
(20)	(1, 0.3)	$\hat{d}$	.000	<b>.710</b>	.290	.000	.000	<b>.985</b>	.015	.000	.105	<b>.895</b>	.000	.000
		$\tilde{d}$	.000	<b>.000</b>	.220	.780	.000	<b>.045</b>	.660	.295	.000	<b>.370</b>	.615	.015
	(3, 0.1)	$\hat{d}$	.005	<b>.535</b>	.450	.010	.085	<b>.845</b>	.070	.000	.545	<b>.455</b>	.000	.000
		$\tilde{d}$	.000	<b>.000</b>	.125	.875	.000	<b>.010</b>	.570	.420	.000	<b>.260</b>	.715	.025
	(3, 0.3)	$\hat{d}$	.000	<b>.535</b>	.465	.000	.015	<b>.895</b>	.090	.000	.185	<b>.815</b>	.000	.000
		$\tilde{d}$	.000	<b>.000</b>	.105	.895	.000	<b>.010</b>	.530	.460	.000	<b>.190</b>	.775	.035

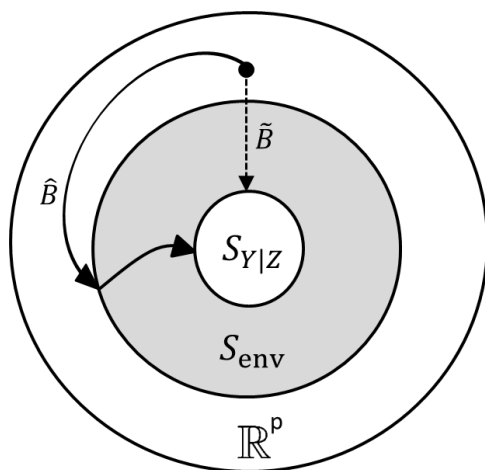


Figure 1: The conceptual display of the two-stage method  $\hat{B}$  (solid line) and the direct method  $\tilde{B}$  (dashed line).

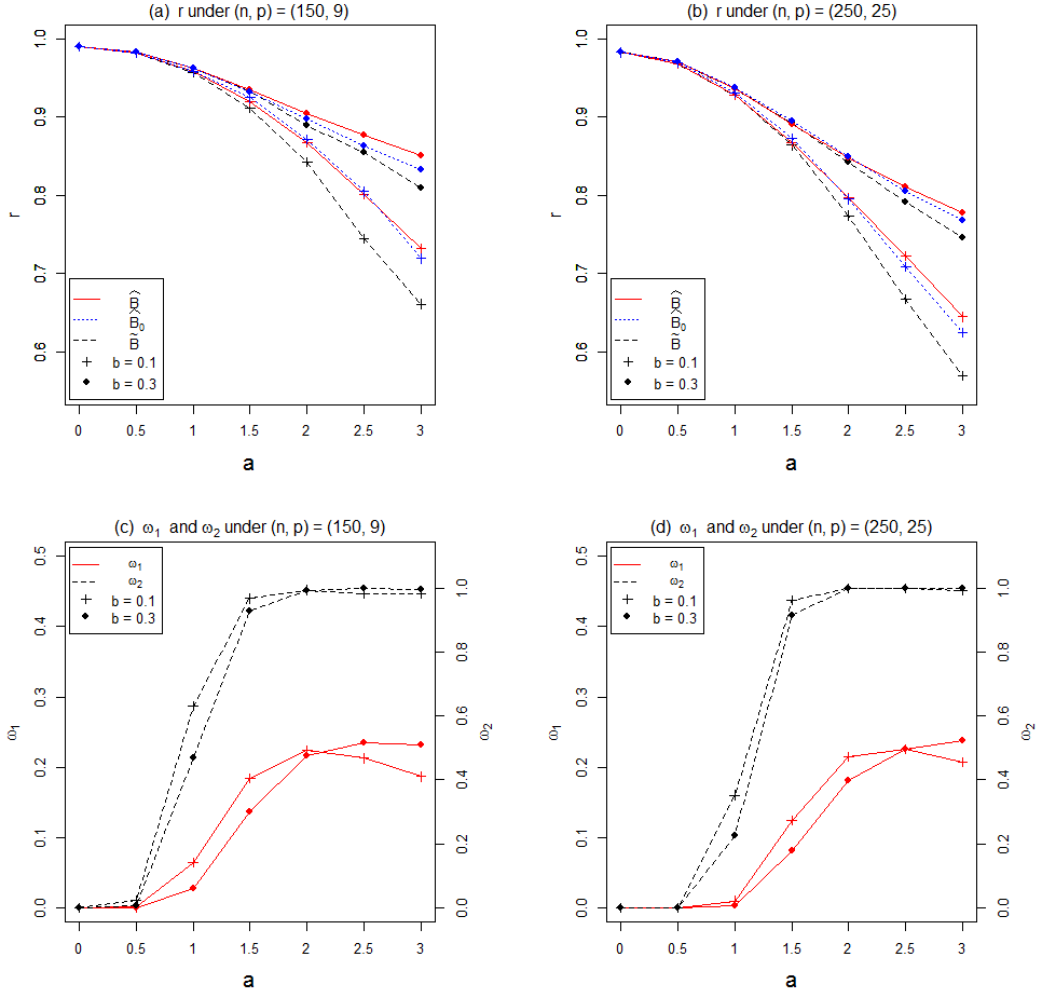


Figure 2: Figures (a)-(b) are trace correlation coefficients and Figures (c)-(d) are variabilities under model (3). The left panels show the case of  $(n, p) = (150, 9)$  and the right panels show the case of  $(n, p) = (250, 25)$ .



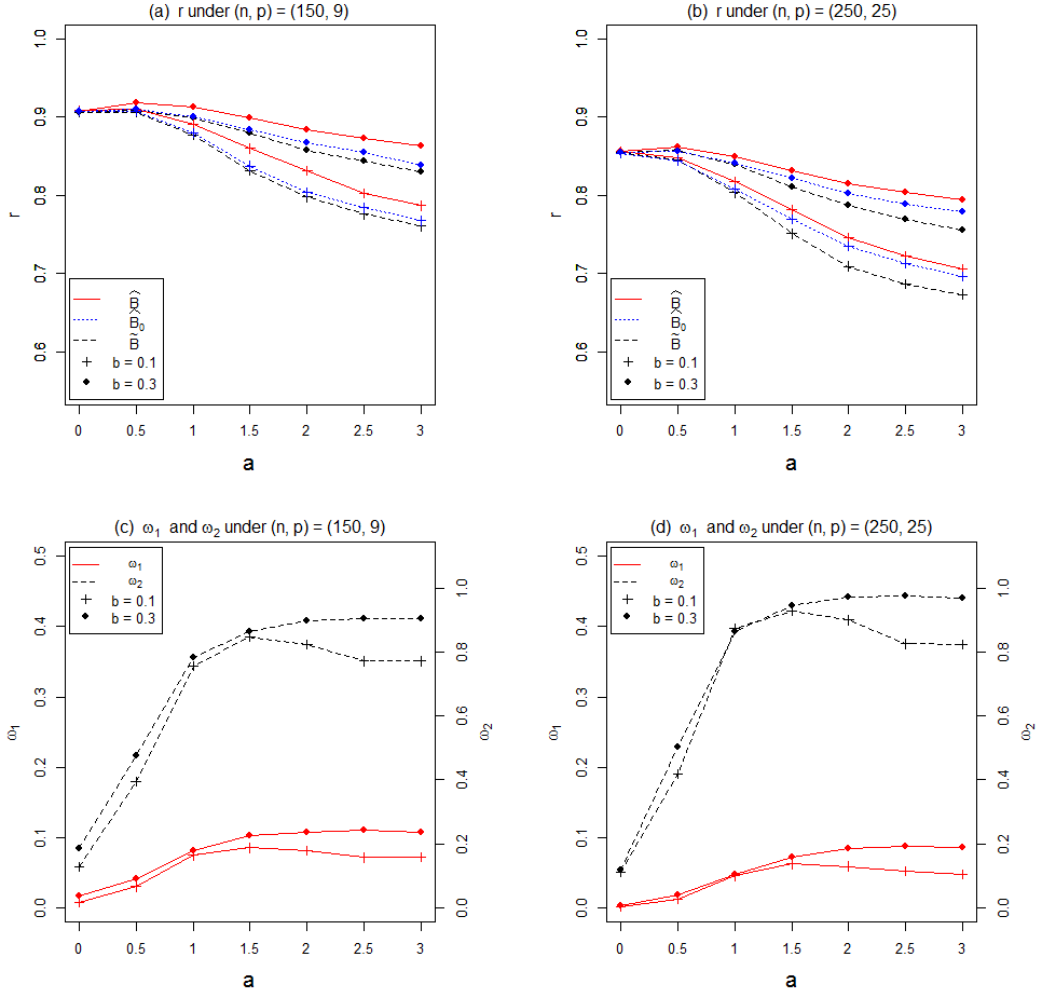


Figure 3: Figures (a)-(b) are trace correlation coefficients and Figures (c)-(d) are variabilities under model (20). The left panels show the case of  $(n, p) = (150, 9)$  and the right panels show the case of  $(n, p) = (250, 25)$ .

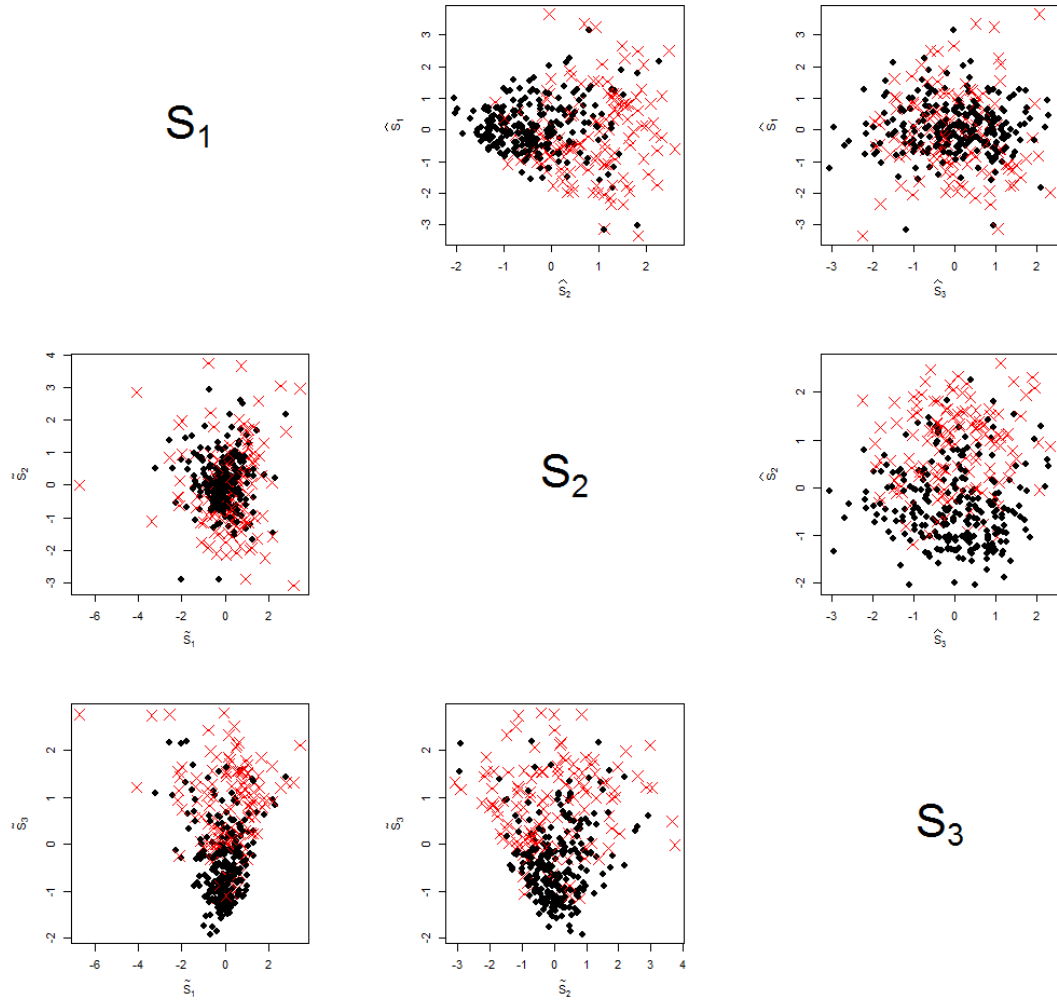


Figure 4: The scatter plot matrix of the leading three extracted predictors from two-stage method in the upper triangular panels, and from direct method in the lower triangular panels.  $\bullet$  and  $\times$  indicate the normal and diabetes patients, respectively